from ICCD. (References 6, 7) On one line per phase it contains an alphabetical listing of elements (by symbol) and the highest ten d-spacings in decreasing order. However it is a polycrystalline database as are the above databases, and therefore the EISI does not include interplanar angles (ϕ). Nor does it include the effects of double diffraction. Its use for polycrystalline electron diffraction is discussed in Reference 6. For single crystal electron diffraction it has the same shortcomings as as the preceding databases with respect to interplanar angles.

NIST Crystal Data, currently in Release J of 1997 on CD-ROM, began in the mid-1980's as a large computer file (first available on tape) of crystallographic and related data obtained from several other original sources: ICDD (then known as The Joint Committee for Powder Diffraction Standards—JCPDS), The Cambridge Crystallographic Centre (U.K.), The Metals Data Center (Ottawa, Canada), The Inorganic Structural Data Center (Germany), and the open literature. Today, the database contains information on 237,659 organic, inorganic, and organometallic phases (of which 79,136 are inorganic) and is available on CD-ROM from NIST or ICDD (References 5, 6, 8). For each phase (also called a "known material", as defined above), the data is organized into sixteen different types of several related fields each (Reference 8). The CD-ROM contains a single flat text file of these types for each phase, plus a coded literature reference file (one of the fields), and various special use files, not used here. There are no d-spacings or any PC software for searching or organizing the data in Release J, 1997, on CD-ROM. However, through its reduced unit cells, this database forms the basis for calculating diffraction patterns in the ZONES database.

In addition, an electron microscopist trained in crystallography might, in favorable circumstances, obtain two zone axis patterns and the interaxial angle between them. NIST has written software to compute the reduced unit cell from this data, which can be searched against the NIST Crystal Data reduced unit cell fields (References 5, 6, 8). This is a powerful and patented (Reference 9) search/match procedure in the hands of a specialist, but it is not as simple as matching three numbers (d_1, d_2, ϕ). There is considerable mathematical complexity in determining reduced unit cell parameters from diffraction data by procedures guaranteed to produce the same ("unique", "conventional") result (from among all the possible permutations) of a, b, c, and of α, β, γ, regardless of which two crystal zone axis patterns are used. It can also be difficult to obtain the required two zone axis patterns and their interaxial angle from the same crystal.

SUMMARY OF THE INVENTION

The present invention is directed to a method for creating a searchable database of crystal electron diffraction data comprising: (a) creating tables within a relational database, said tables comprising Code data, Formula data, and Element data; wherein said Code data includes information relating to the d-spacings and acute angles of diffraction patterns of crystals, said Formula data includes information relating to the chemical formulae of said crystals, and said Element data includes information relating to the presence of elements of high atomic number in said crystals; (b) creating at least one macro for performing searches using said tables; said at least one macro including the steps of: (i) requesting input data relating to observed d-spacings, acute angles, experimental error limits, and anticipated atomic numbers of an experimental sample; (ii) comparing said input data with the data in said tables in accordance with said experimental error limits; and (iii) generating at least one report listing the crystals within said tables that match said input data.

The invention is also directed to a method for classifying crystal electron diffraction data obtained from an experimental sample, comprising: (a) generating a relational database comprising: (i) at least three tables holding Code data, Formula. data, and Element data, respectively; wherein said Code data includes information relating to the d-spacings and acute angles of diffraction patterns of crystals, said Formula data includes information relating to the chemical formulae of said crystals, and said Element data includes information relating to the presence of elements of high atomic number in said crystals; (ii) at least one macro for performing searches using said tables; said at least one macro including the steps of: (1) requesting input data relating to observed d-spacings, acute angles, experimental error limits, and anticipated atomic numbers of an experimental sample; (2) comparing said input data with the data in said tables in accordance with said experimental error limits; and (3) generating at least one report listing the crystals within said tables that match said input data; and (b) using said macro of said relational database to enter electron diffraction data obtained from said experimental sample and to obtain said at least one report.

The invention also provides a relational database for classifying crystal electron diffraction data obtained from an experimental sample, said database comprising: (a) at least three tables holding Code data, Formula data, and Element data, respectively; wherein said Code data includes information relating to the d-spacings and acute angles of diffraction patterns of crystals, said Formula data includes information relating to the chemical formulae of said crystals, and said Element data includes information relating to the presence of elements of high atomic number in said crystals; (b) at least one macro for performing searches using said tables; said at least one macro including the steps of: (i) requesting input data relating to observed d-spacings, acute angles, experimental error limits, and anticipated atomic numbers of an experimental sample.; (ii) comparing said input data with the data in said tables in accordance with said experimental error limits; and (iii) generating at least one report listing the crystals within said tables that match said input data.

DETAILED DESCRIPTION OF THE INVENTION

The present invention provides the construction and searching of a relational database of values d_1, d_2, and ϕ, plus coded elemental composition, for known crystalline solids. Through the use of new software and computational methods and procedures associated with this relational database, unknown materials are matched to 79,136 inorganic compounds in embodiment.

The present invention provides the following advantages: (1) it permits an electron microscopist with little or no training in crystallography, and (2) only elementary training in common personal computer (PC) software tools to (3) identify the substance or substances which produced a single crystal electron diffraction pattern from (4) among as wide as possible a set of "knowns". In the present invention, identification of all inorganic materials in the NIST Crystal Data file, in (5) less than 14 seconds search time (the common limit of human patience in such matters)is accomplished.

All of the above five advantages are met with the present invention. Unique features of this invention not found elsewhere are: (1) Rational inclusion in the database of specific d-spacings which produce spots by "double diffraction"